# PROTEIN MODELING

**Read the General Rules in the manuals and on www.soinc.org as they apply to every event.**

1. **DESCRIPTION:** Students will use computer visualization and online resources to guide them in constructing physical models of proteins. For the 2011 competitions, students will model proteins involved in reprogramming adult cells to become stem cells, also known as induced pleuripotent stem cells (IPS).
   **A TEAM OF UP TO:** 3 **IMPOUND:** Yes **APPROXIMATE TIME:** 50 minutes for **Part II & III**
2. **EVENT PARAMETERS:** Pre-build models will be impounded one hour before the event begins.
   a. Students may bring up to five double-sided, 8.5"x11" pages of notes. Internet access is not permitted.
   b. Students must bring a writing instrument.
   c. Supervisors will provide all materials for on-site model construction.
3. **THE COMPETITION:** This event has three parts: a pre-build model, an on-site build model, & an exam.
   a. **Part I: The Pre-Build Model.** Students will use a computer visualization program (Jmol; http://cbm.msoe.edu/includes/jmol/SOJmols/2011PreBuild.html) to design and construct a model of a specific protein based on atomic coordinate data. Students will construct a model of Klf4, based on the coordinate data found in the 2wbu.pdb file. Structural information about this file can be accessed for free through the RCSB Protein Data Bank (www.pdb.org). The same constructed model of the Klf4 protein will be brought to all competitions; as the competition level increases, the scoring rubrics for the pre-build model will reflect higher expectations for model accuracy, detail and creativity.
   b. The final pre-build model must be based on the alpha carbon backbone display of the model and must use a scale of 2 cm per amino acid. Students may use Mini-Toobers® to model their protein, or use other comparable material (e.g., Kwik Twists, 12 gauge dimensional house wire, etc.). Students will represent other important parts of the protein, such as amino acid sidechains, DNA or associated molecules, with materials of their choosing. The additions to the model should focus on illustrating the significance of the structure to the function of the protein. A significant portion of the score will be derived from the creative additions to the model. Students must provide a 3"x5" note card explaining the additions to their model and what they represent. Students must deliver their pre-build model and 3"x5" card to judges at the competition site for impounding. Models will be returned to the students after the competition.
   c. **Part II: The On-Site Model.** During the on-site competition at Regional Competitions, students will design and build a physical model of a selected region of Oct4 (1gt0.pdb), which is described in the April 2009 *RCSB Molecule of the Month* (http://dx.doi.org/10.2210/rcsb_pdb/mom_2009_4) by David S. Goodsell. During the on-site competition at the State Competition, students will design and build a physical model of a selected region of Nanog (2kt0.pdb). During the on-site competition at the National Competition, students will design and build a physical model of a selected region of c-myc (1nkp.pdb), which is described in the April 2009 *RCSB Molecule of the Month* (http://dx.doi.org/10.2210/rcsb_pdb/mom_2009_4) by David S. Goodsell.
   d. Students will utilize a computer provided with the Jmol application at the competition. Students must utilize only one of the identical computers provided at the competition with the above-mentioned files on it to guide their model construction. All construction materials for the model (Mini-Toobers®[1], foam amino acid sidechains, crosslinkers and plastic red and blue end caps) will be provided. Any model not handed to the judges by the end of the competition time will not be accepted for scoring.
   e. **Part III: The On-Site Written Exam** will be multiple choice/short answer questions about the relationship between protein structure and function, with an emphasis on induced pleuripotent stem cells.
4. **SCORING:** 40% of the event score will be based on the pre-build protein model (Part I), 30% on the on-site build (Part II) and 30% on the written exam (Part III). The pre-build protein model (Part I) will be scored based on the accuracy & scale of the alpha-helix & beta-sheet secondary structures, as well as other creative additions to the protein backbone such as sidechains, DNA or associated molecules. The focus of the model should be on creatively telling the story of the molecule's significance, structure & function. Creative additions that do not support the molecular story will not receive full credit. The on-site build protein model (Part II) will be scored based on accuracy of folding the Mini-Toober® model & positioning specific amino acid sidechains and/or accessory molecules. The exam (Part III) will be scored for accuracy. Ties will be broken using specific questions from the written exam selected by the event supervisor.

**Resources:** Event details and available kit information can be found at: http://cbm.msoe.edu/stupro/so/index.html

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